

Alloying Solid Solution Strengthening of Fe-Ga Alloys:

A first-principles Study

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Abstract

First-principles spin polarized calculations have been implemented by using the Discrete Molecular (DMol3) package to investigate the strengthening effect from alloying additions of Nb, Mo, V, Cr and Co in cubic solid solution of Fe-Ga alloys. Mayer bond order (BO) values were used to evaluate the atomic bond strengths in the alloys, and were then used to assess the alloying strengthening characteristics. Results from the calculation suggested that transition metal Nb achieves the best strengthening effect in Fe-Ga alloys. The solid solution strengthening follows a trend from larger to smaller by Nb, Mo, V, Cr and Co. The effect of Ga on individual bond strength variation between Fe and alloying elements and also on alloying strengthening was examined.

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Magnetostrictive materials are widely used for sensor and actuator device applications. It has been recognized that substituting a small amount of non-magnetic Ga element for Fe in bcc solid solution results in an unprecedented ten-fold increase in magnetostriction ($3/2\lambda_{100}$) over that of Fe and twice the increase compared to FeAl alloys [1,2]. Fe-Ga alloys are found to become elastically very soft at certain composition range, and the softening of the shear elastic constant $\frac{1}{2}(C_{11}-C_{12})$ is believed to explain the novel magnetostrictive behavior of the alloys [3]. In addition to the magnetostrictive properties, an enhancement of mechanical properties, such as solid solution strengthening in Fe-Ga alloys with specifically chosen alloying elements, is another important issue in the development of Fe-Ga alloys. Thus, a thorough investigation of the underlying mechanism responsible for alloying strengthening is essential to the research on Fe-Ga alloys. Currently, obtaining an alloy with both good toughness as well as novel magnetostrictive properties still remains a challenge. To our knowledge, there are no direct experimental or theoretical studies on the strengthening mechanism associated with alloying additions of Nb, Mo, V, Cr and Co in Fe-Ga alloys. In this study, we make a first effort to investigate the mechanism of solid solution strengthening of Fe-Ga alloys by first principles calculations. To this end, fully quantum-mechanical cluster calculations have been performed using the DMol3 molecular orbital package. The information achieved in this study is expected to provide guidance in the design of Fe-Ga alloys.

As a molecular cluster approach, DMol3 package is based on the density functional theory [4]. Double numerical basis sets are employed in spin polarized calculations. The

degree of convergence of the self-consistent iterations, measured by (r.m.s.) changes in the charge density, was set to be 10^{-5} , which allowed the energy to converge to 10^{-5} Ryd. All calculations in the present research were performed with the generalized-gradient approximation (GGA) proposed by Perdew and Wang [5]. In order to quantitatively investigate the alloying strengthening effect, the atomic bond strength between atoms was first calculated. In this study, the atomic bond strength is measured by Mayer bond order, a measure of the overlap of electron wavefunctions of atoms. The Mayer bond order (BO) between atoms A and B is defined as follow [6]:

$$BO_{AB} = 2 \sum_{\mu \in A} \sum_{\nu \in B} [(P^\alpha S)_{\mu\nu} (P^\alpha S)_{\nu\mu} + (P^\beta S)_{\mu\nu} (P^\beta S)_{\nu\mu}] \quad (1)$$

where P^α , P^β are the density matrices and S is the overlap matrix of the wavefunctions [6]. Bond order values were evaluated within the first nearest neighbor (FNN) distance of atoms. The calculations indicate that if the separation between atoms A and B is beyond the FNN range, the BO_{AB} value is small and can be neglected. This approach has recently been successfully applied in alloying strengthening study of Ni-base alloys [7-9]. In order to clarify the bond enhancement effect, a new parameter $\Delta BO(X, X_0)$ is defined as:

$$\Delta BO(X, X_0) = BO(X) - BO(X_0) \quad (2)$$

where $BO(X_0)$ is the bond strength between element X_0 and its FNN in an alloy, while $BO(X)$ is the bond strength when element X_0 is substituted by element X. If $\Delta BO(X, X_0) > 0$, then the element X has an ability to enhance the atomic bond strength. The larger $\Delta BO(X, X_0)$ is, the greater effect the element X achieves on enhancing atomic bond strength. Furthermore, a new parameter $\sum \Delta BO$ that is defined as

$$\sum \Delta BO = \sum BO(X) - \sum BO(X_0) \quad (3)$$

is then used to evaluate the alloying strengthening effect. In Eq (3), ΣBO represents a local BO summation within the FNN, which represents a typical solid solution strengthening through local bond characteristics.

To study solid solution strengthening, the effect of individual bond strength and the alloying addition on bond strength variation were examined. Figure 1 shows a cubic cluster model of Fe with 35 atoms in size used for BO calculations. This model is large enough so that the surface effect on bond strength between Fe(1) (at the center of the model) and its first neighbors can be neglected [9]. For a cluster with bcc symmetry as shown in Figure 1, there are 8 first nearest neighbor atoms surrounding the Fe(1) site. To reveal the underlying mechanism and effect of alloying strengthening in Fe-Ga alloys, the following situations were taken into account:

1. A pure Fe cluster to study the bond strength between Fe(1) and other Fe atoms within the FNN range;
2. Substituting one X(1) atom ($X = \text{Nb, Mo, V, Cr and Co}$) for Fe(1) to study the bond strength variation between X(1) and Fe atoms within FNN range;
3. Following (2), substituting one Ga atom for Fe located at the FNN range of X(1) to study the effect of a Ga atom on the bond strength between X(1) and Fe(X);
4. Following (3), substituting one more Ga atom for another Fe atom located at the FNN of X(1) to further study the change in bond strength by the present of 2 Ga atoms;

5. Evaluating the bond strength between Ga(1) and other Fe atoms without any other alloying additions.

The information on bond strength from situations (1) to (5) was then used to assess the effect of X addition on solid solution strengthening in Fe-Ga alloys. Tables 1, 2 & 3 present the calculated bond strengths measured by Mayer bond order values derived from equations (1) to (3).

Tables 1 & 2 show that the atomic bond strength BO^{Fe-X} (X = Nb, Mo, V, Cr, Co) due to alloying addition in pure Fe cluster follows a trend as:

$$BO^{Fe-Nb} > BO^{Fe-Mo} > BO^{Fe-V} > BO^{Fe-Cr} > BO^{Fe-Co} > BO^{Fe-Ga} > BO^{Fe-Fe} \quad (4)$$

Similarly, from equation (3), the alloying strengthening effect in Fe, without the present of Ga, follows as:

$$\sum BO_{FeNb} > \sum BO_{FeMo} > \sum BO_{FeV} > \sum BO_{FeCr} > \sum BO_{FeCo} > \sum BO_{FeFe} \quad (5)$$

Therefore, these results suggest that among the elements considered, the transition metal Nb achieves the best solid solution strengthening effect in cubic Fe. In the case where one Ga atom substitutes for Fe, the individual atomic bond strength was altered to some extent (see Table 1). The variation of individual bond strength due to the addition of 1 or 2 Ga atoms to the FNN range follows such a trend as:

$$BO_{Fe2GaX}^{Fe-X} > BO_{FeGaX}^{Fe-X} > BO_{FeX}^{Fe-X} \quad (6)$$

The subscripts in equation (6) for BO represent the cases considered in Table 1, while the superscripts indicate the atomic bond between Fe and X atoms. Tables 1 and 2 show that the extent of solid solution strengthening due to alloying addition as follows:

$$\sum BO_{FeGaNb} > \sum BO_{FeGaMo} > \sum BO_{FeGaV} > \sum BO_{FeGaCr} > \sum BO_{FeGaCo} \quad (7)$$

This trend holds for the situation where two Ga atoms present in the cluster model:

$$\sum BO_{Fe2GaNb} > \sum BO_{Fe2GaMo} > \sum BO_{Fe2GaV} > \sum BO_{Fe2GaCr} > \sum BO_{Fe2GaCo} \quad (8)$$

It indicates that although the individual bond strength was modified (either enhanced or reduced) due to the present of Ga atoms, the trend of alloying strengthening remains the same.

Furthermore, the variation of bond strength between X and Ga (Table 3) shows a different trend compared to that between X and Fe:

$$BO_{FeGaMo}^{Mo-Ga} > BO_{FeGaNb}^{Nb-Ga} > BO_{FeGaCr}^{Cr-Ga} > BO_{FeGaV}^{V-Ga} > BO_{FeGaCo}^{Co-Ga} \quad (9)$$

and

$$BO_{Fe2GaMo}^{Mo-Ga} > BO_{Fe2GaNb}^{Nb-Ga} > BO_{Fe2GaCr}^{Cr-Ga} > BO_{Fe2GaCo}^{Co-Ga} > BO_{Fe2GaV}^{V-Ga} \quad (10)$$

In addition, for all the additional elements considered (except for Co), the alloying solid solution strengthening effect follows the same trend, as shown in Table 2:

$$\sum BO_{FeX} > \sum BO_{FeGaX} > \sum BO_{Fe2GaX} \quad (11)$$

These results indicate that the solid solution strengthening effect decreases with increase in Ga content.

In conclusion, by carrying out first-principles spin polarized calculations using the DMol3 package, we observed that, among Nb, Mo, V, Cr and Co, transition metal Nb achieves the best solid solution strengthening effect in cubic Fe. Although addition of Ga

modifies the individual bond strength between Fe and alloying elements to some extent, the trend on strengthening due to alloying addition remains the same.

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Figure captions

Figure 1. The cubic 35-atom cluster model of Fe for bond strength calculations. The larger grey circle at the center (0,0,0) in the model represents Fe atom and was substituted by alloying metals X (X = Nb, Mo, V, Cr and Co) to study alloying strengthening effects. The eight smaller grey circles represent the first nearest neighbor atoms of the center atom, and these neighbor atoms were substituted by Ga atoms to simulate Ga effects on bond strength variation and also on alloying strengthening effect.

Figure 1.

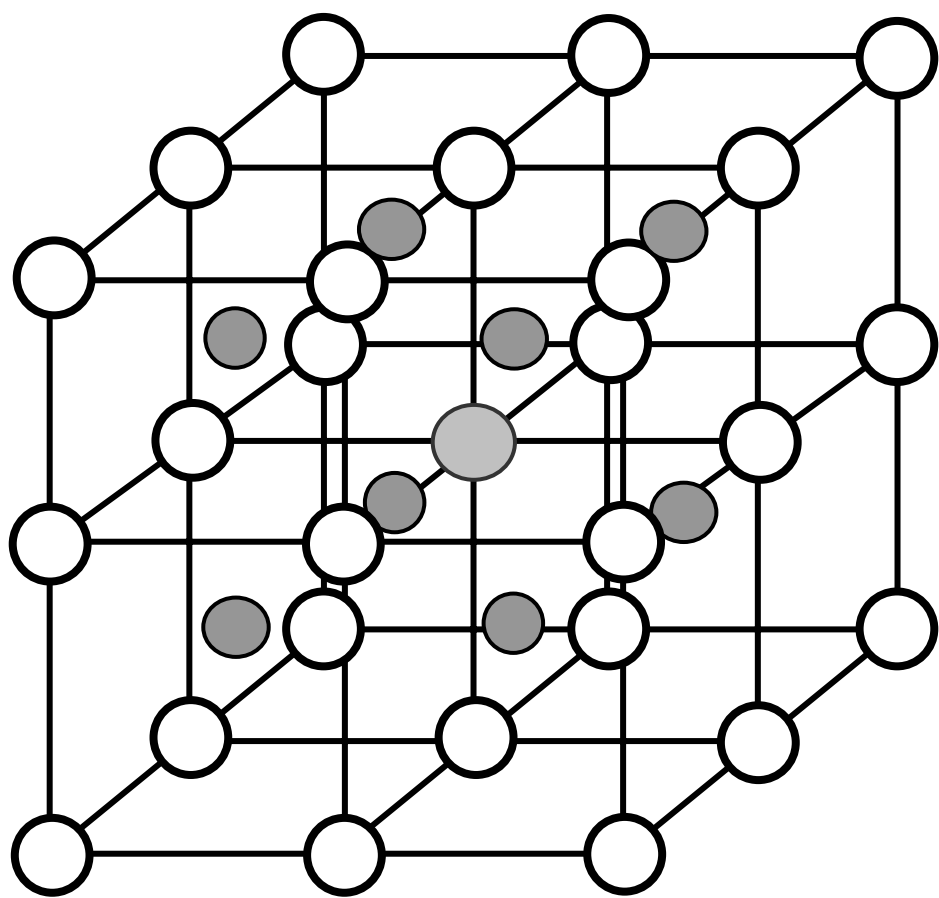


Table 1. The calculated individual bond strength BO^{Fe-X} between Fe and alloying element X (X = Nb, Mo, V, Cr and Co) in pure Fe (case 2), FeGa (case 3) and Fe2Ga (case 4) systems.

	BO^{Fe-Nb}	BO^{Fe-Mo}	BO^{Fe-V}	BO^{Fe-Cr}	BO^{Fe-Co}
FeX	0.5332	0.5292	0.4743	0.4437	0.2955
FeGaX	0.5338	0.5302	0.4779	0.4469	0.2999
Fe2GaX	0.5505	0.5427	0.4898	0.4554	0.2999

Table 2. Alloying strengthening effects represented by bond strength summation $\sum BO^{Fe-X}$ in pure Fe (case 2), FeGa (case 3) and Fe2Ga (case 4) system.

	$\sum BO^{Fe-Nb}$	$\sum BO^{Fe-Mo}$	$\sum BO^{Fe-V}$	$\sum BO^{Fe-Cr}$	$\sum BO^{Fe-Co}$
Fe	4.2656	4.2416	3.7944	3.5488	2.3642
FeGaX	4.0441	4.0247	3.6209	3.4168	2.3802
Fe2GaX	3.9454	3.9186	3.4808	3.2948	2.3488

Table 3. The individual bond strength between Ga and alloying element X (X = Nb, Mo, V, Cr and Co).

	$\text{BO}^{\text{Ga-Nb}}$	$\text{BO}^{\text{Ga-Mo}}$	$\text{BO}^{\text{Ga-V}}$	$\text{BO}^{\text{Ga-Cr}}$	$\text{BO}^{\text{Ga-Co}}$
FeGaX	0.3075	0.3203	0.2756	0.2885	0.2747
Fe ₂ GaX	0.3203	0.3312	0.271	0.2802	0.2747